are present.

[13]We find $B = 1.47 \pm 0.15$ and $2 - B' = 1.8 \pm 0.2$ at $T = 1.3$ K. These agree within our mutual uncertainties, with an extrapolation of the data in P. Lucas, J. Phys. C 3, 1180 (1970), to our temperature.

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# Theory of the Neutron Scattering Cross Section in Spin-Glasses

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Using mean-field theory we compute the frequency-integrated neutron cross section $I(q,T)$ for spin-glasses. We find, as observed experimentally, that the temperature of the maximum of $I(q,T)$ depends on the momentum transfer $q$ and is different from the freezing temperature $T_c$ at which the susceptibility $\chi(q,T)$ has a cusp. These results suggest that recent neutron scattering experiments are consistent with a sharp phase transition at a single temperature $T_c$ in spin-glasses.

Among the more puzzling experimental results concerning the concentrated spin-glass alloys are Murani's recent neutron scattering measurements,[1] which show that the frequency-integrated scattering intensity $I(q, T)$ has a temperature-dependent maximum which varies with momentum transfer $q$. These data have been interpreted[1] as suggesting that there is no unique freezing temperature in these alloys, associated with the spin-glass phase. Rather, the system is viewed as subdivided into correlated, ferromagnetic clusters, which freeze at different temperatures depending on their characteristic size.

The purpose of the present Letter is to show that these neutron experiments *are* consistent with the theory that there is a sharp phase transition in the spin-glasses. This is demonstrated in two different ways based on (i) a simple data analysis and (ii) a mean-field random-phase-approximation (RPA) calculation of the neutron scattering cross section, appropriate to concentrated spin-glasses.

The frequency-integrated neutron scattering cross section is given by[2]

$$\frac{d\sigma}{d\Omega_q} = \frac{N}{\hbar}\left(\frac{\gamma e^2}{mc^2}\right)^2 \frac{k'}{k} |F(q)|^2 I(q, T). \tag{1}$$

Here $N$ is the number of scattering sites, $k$ and $k'$ are the incident and final wave vectors of the neutron, $\gamma e^2/mc^2$ is the coupling constant, and $F(q)$ is the scattering form factor which varies on a scale characteristic of atomic dimensions. The quantity $I(q, T)$ is given by

$$I(q, T) = N^{-1} \sum_{i,j} [\langle \vec{S}_i \cdot \vec{S}_j \rangle]_c \exp[i\vec{q} \cdot (\vec{R}_i - \vec{R}_j)], \tag{2}$$

where $[\,]_c$ denotes a configuration average and it is assumed that, consistent with experiment,[1] the magnetic contribution dominates that of potential scattering. $I(q, T)$ is generally written as

$$I(q, T) = k_B T \chi(q, T) + I_B(q, T), \tag{3}$$

where $k_B$ is the Boltzmann's constant. We thus define

$$k_B T \chi(q, T) \equiv N^{-1} \sum_{i,j} \{[\langle \vec{S}_i \cdot \vec{S}_j \rangle]_c - [\langle \vec{S}_i \rangle \cdot \langle \vec{S}_j \rangle]_c\} \exp[i\vec{q} \cdot (\vec{R}_i - \vec{R}_j)], \tag{4a}$$

and

$$I_B(q, T) \equiv N^{-1} \sum_{i,j} [\langle \vec{S}_i \rangle \cdot \langle \vec{S}_j \rangle]_c \exp[i\vec{q} \cdot (\vec{R}_i - \vec{R}_j)]. \tag{4b}$$

This last term plays a role analogous to the Bragg scattering term in ordinary ferromagnets, whereas the first is the wave-vector–dependent susceptibility.[3] In periodic ferromagnets, away from the reciprocal-lattice vectors $I_B(q, T) = 0$. By contrast, for spin-glasses, this term is very important.

In the Edwards-Anderson[4] (EA) mean-field theory, the spin-glass order parameter is $\overline{Q}_{ij} \equiv [\langle \vec{S}_i\rangle \cdot \langle \vec{S}_j\rangle]_c$. Thus, $I_B(q, T)$ is the Fourier transform of the order parameter. While $\overline{Q}_{ij} \propto \delta_{ij}$ in the EA theory, it is reasonable to assume more generally that this order parameter has some finite spatial extent which reflects the characteristic range of the direct (ferromagnetic) spin-spin correlation. Because $I_B(q, T)$ represents an order parameter, it decreases monotonically to zero as $T$ approaches the freezing temperature $T_c$. The term $T\chi(q, T)$ is expected to have a sharp maximum at $T_c$ and the sum of these two contributions can then lead to a maximum in $I(q, T)$ which occurs at a $q$-dependent temperature $T_0(q) < T_c$, as is observed experimentally.[1]

In Fig. 1, we illustrate how the above remarks are consistent with experimental data[1] on a rather

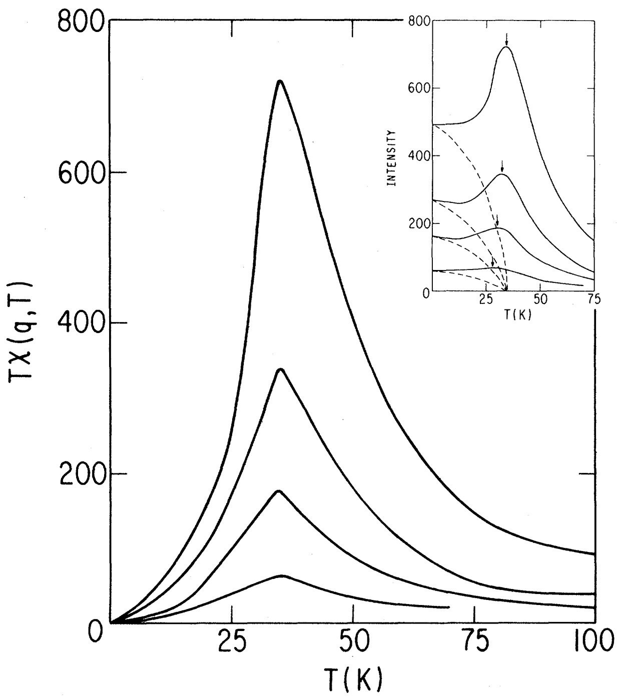


FIG. 1. The wave-vector–dependent susceptibility $T\chi(q,T)$ in an $Au$Fe alloy deduced by subtracting an estimate of the "Bragg" term (dashed) from the measured (Ref. 1) total cross section $I(q,T)$ (plotted in the inset). Values of $q$ were 5.2, 6.9, 8.6, and 13.8 $\times 10^{-3}$ Å$^{-1}$ from top to bottom.

concentrated 10% $Au$Fe spin-glass. The inset shows the experimental measurements[1] of $I(q, T)$, indicated by solid lines. The dashed lines represent estimates of the "Bragg" contributions at each $q$. These are obtained by drawing smooth monotonic curves through the known points $I_B(q, 0) = I(q, 0)$ and $I_B(q, T_c) = 0$. It should be noted from the data that $I_B(q, 0) = I(q, 0)$ is strongly $q$ dependent. This confirms the notion that the EA order parameter has some spatial extent. To be consistent with direct measurements of the spin-glass order parameter,[5] as well as with calculations to be described below, we chose $I_B(q, T)$ so that the exponent $\beta$ is less than 1. The range of acceptable values of $T_c$ has as its lower bound the maximum $T_0(q)$, which is $33 \pm 1$ K, and can be a few degrees above it. We choose $T_c = 35$ K. This is consistent with $T_c = 35 \pm 5$ K found by other investigators[6] for alloys of the same concentration. The result of the subtraction, $[I(q, T) - I_B(q, T)]$, is illustrated in Fig. 1. As expected, all the $T\chi(q, T)$ curves have their maximum at $T_c$, consistent with mean-field theory. This interpretation of the data is, clearly, not definitive, but it is, nevertheless, extremely suggestive of the fact that the neutron measurements are *not* inconsistent with a sharp phase transition in the spin-glasses.

We now extend the EA mean-field theory to compute $I(q, T)$. We use a cluster decomposition of the EA model Hamiltonian to include some of the direct ferromagnetic interactions expected in a concentrated spin-glass like $Au_{0.9}Fe_{0.1}$ and to be consistent[7] with specific-heat data,

$$\mathcal{H} = -\sum_{\nu<\lambda} J_{\nu\lambda}\vec{S}_\nu \cdot \vec{S}_\lambda - \sum_{\nu}\sum_{i<j} J_{ij}{}^0 \vec{S}_{i\nu} \cdot \vec{S}_{j\nu}. \qquad (5)$$

This model, which was introduced earlier[7] to discuss the behavior of the thermodynamic properties of the spin-glasses, contains both intracluster interactions (with ferromagnetic exchange constant $J_{ij}{}^0$) as well as intercluster interactions (with random exchange constant $J_{\nu\lambda}$). The former are treated exactly whereas the latter which represent the weaker interactions between far-away spins are computed in random–mean-field theory. Greek indices refer to a particular cluster and Roman indices to a given spin within that cluster. Here $\vec{S}_\nu = \sum_i \vec{S}_{i\nu}$. The present theory may be viewed as a way of treating the simplest type of fluctuation corrections to mean-field theory: The clusters represent those spins between which the exchange interactions are too strong to be treated adequately by mean-field theory.

We take $J_{\nu\lambda}$ to be a near-neighbor interaction distributed with probability

$$P(J_{\nu\lambda}) = (1/\sqrt{2\pi}J)\exp[-(J_{\nu\lambda}-J_{\nu\lambda}')^2/2J^2],$$

where $J'$ is the net ferromagnetic intercluster exchange interaction. Using the replica method we compute the intracluster variational parameters $[\langle \vec{S}_i \cdot \vec{S}_j\rangle]_c \equiv M_{ij}$ and $[\langle \vec{S}_i\rangle \cdot \langle \vec{S}_j\rangle]_c \equiv Q_{ij}$ for an average cluster of $\overline{N}$ spins. The effects of including a distribution of cluster sizes are discussed below. Here $i$ and $j$ belong to the same ($\nu$th) cluster; $\sum_{i,j} M_{ij}(T)$ is the cluster moment $M(T)$ and $\sum_{i,j} Q_{ij}(T) \equiv Q(T)$ is the intracluster contribution to the order parameter.[7] $M \equiv M(T)$ and $Q \equiv Q(T)$ were discussed in an earlier paper.[7] Following Refs. 7 and 8, we have

$$M_{ij}(T) = (2\pi)^{-3/2}\int d^3r\, e^{-r^2/2}\mathrm{Tr}[\vec{S}_{i\nu}\cdot \vec{S}_{j\nu}e^{-\beta H^{\mathrm{eff}}}]Z^{-1}, \tag{6}$$

and

$$Q_{ij}(T) = (2\pi)^{-3/2}\int d^3r\, e^{-r^2/2}\mathrm{Tr}[\vec{S}_{i\nu}e^{-\beta H^{\mathrm{eff}}}]\cdot \mathrm{Tr}[\vec{S}_{j\nu}e^{-\beta H^{\mathrm{eff}}}]Z^{-2}, \tag{7}$$

where

$$-H^{\mathrm{eff}} = \sum_{i<j} J_{ij}{}^0\vec{S}_{i\nu}\cdot\vec{S}_{j\nu} + \bar{J}(\tfrac{1}{3}Q)^{1/2}\vec{r}\cdot\vec{S}_\nu + \tfrac{1}{6}\bar{J}^2\beta(M-Q)\vec{S}_\nu\cdot\vec{S}_\nu + \vec{S}_\nu\cdot\sum_{\lambda\neq\nu} J_{\nu\lambda}'\langle\vec{S}_\lambda\rangle.$$

Here $Z = \mathrm{Tr}e^{-\beta H^{\mathrm{eff}}}$ and $\bar{J} \equiv z^{1/2}J$, with $z$ equal to the number of cluster mean neighbors of a given cluster and $\beta = (k_B T)^{-1}$.

The susceptibility $\chi(q,T)$ is computed by including a magnetic field term $\sum \vec{H}_j\cdot\vec{S}_j$ in $H^{\mathrm{eff}}$ and differentiating the induced local moment $\langle\vec{S}_i\rangle$ with respect to $H_j$. We find after straightforward algebra that, for $J_1(q) \equiv \sum_\nu J_{\nu\lambda}'\exp[i\vec{q}\cdot(\vec{R}_\nu - \vec{R}_\lambda)]$,

$$k_B T\chi(q,T) = [M(q,T) - Q(q,T)]/\{1 - \beta J_1(q)[M(q,T) - Q(q,T)]\}, \tag{8}$$

where

$$M(q,T) = \sum_{i,j\in\nu} M_{ij}(T)\exp[i\vec{q}\cdot(\vec{R}_i - \vec{R}_j)]$$

and $Q(q,T)$ is defined analogously. As was expected, this result is of the generalized Ornstein-Zernike form. In the limit in which $M$ and $Q$ are independent of $q$, Eq. (8) was suggested by earlier workers.[9] The intercluster "Bragg-like" contribution to $I(q,T)$ can be similarly derived by expanding $[\langle\vec{S}_{k\delta}\rangle\cdot\langle\vec{S}_{i\nu}\rangle]_c$ for $\nu\neq\delta$ to lowest order in $J'$ and factorizing the configuration average of the product into the product of the averages. This yields the expected RPA-like result

$$[\langle\vec{S}_{k\delta}\rangle\cdot\langle\vec{S}_{i\nu}\rangle]_c = \beta\sum_{\substack{l\in\nu\\ j\in\lambda}}\{\sum_{\lambda\neq\delta} J_{\nu\lambda}'[\langle\vec{S}_{k\delta}\rangle\cdot\langle\vec{S}_{j\lambda}\rangle]_c(M_{il} - Q_{il}) + J_{\nu\delta}'[\langle\vec{S}_{k\delta}\rangle\cdot\langle\vec{S}_{j\delta}\rangle]_c(M_{il} - Q_{il})\}, \tag{9}$$

where $l$ and $j$ range only over sites within a particular cluster. Upon taking the Fourier transform and adding the intracluster contribution $Q(q,T)$ we find

$$I_B(q,T) = Q(q,T)/\{1 - \beta J_1(q)[M(q,T) - Q(q,T]\}. \tag{10}$$

Note that (i) $I_B(q,T)$ is zero for $T \geq T_c$ and that (ii) the characteristic range of the direct ferromagnetic interactions leads to a $q$ dependence in $I_B(q,T)$ through both the intracluster and intercluster interactions. Equation (10) for the case in which $Q$ and $M$ are $q$ independent and $T\approx T_c$ was derived elsewhere.[10] Combining Eqs. (8) and (10) gives

$$I(q,T) = M(q,T)/\{1 - \beta J_1(q)[M(q,T) - Q(q,T)]\}. \tag{11}$$

We have investigated the $T$ dependence of Eq. (11) for a range of models. It can be shown analytically that for rigid, giant Heisenberg spins (in which $dM/dT = 0$) $I(q,T)$ has a maximum at $T_c$. We find from a systematic numerical analysis that $I(q,T)$ *will always have a maximum below* $T_c$, *for both Heisenberg and Ising spins, whenever* (i) $dM/dT\neq 0$ *and* (ii) $J\neq 0$. These results are insensitive to the detailed $q$ dependence of $M$ and $Q$, so that the cluster configuration and size are irrelevant parameters. The cluster model is only necessary in order to obtain a temperature dependence in $M$.

For definiteness we illustrate these general remarks with a particular example. We consider an average cluster size of $\overline{N}=10$ Ising spins which interact ferromagnetically with their near neighbors. This represents essentially the largest cluster for which Eqs. (6) and (7) can be numerically evaluated. The use of Ising rather than Heisenberg spins was necessary in order to treat the maximum possible $\overline{N}$. We chose $|\overline{J}/J_0| \sim 0.01$ to yield reasonably good agreement with the specific heat $C_m$ temperature dependence.[7] As in Ref. 7 it was found that both $C_m$ and $\chi(0,T)$ were in semiquantitative quantitative agreement with experiment. For simplicity, we choose to place the cluster spins in a one-dimensional array with $\vec{q}$ parallel to the cluster and we took $J_1(q)/J_0 = (0.008-0.01)(qa)^2$, where $a$ is the characteristic spin-spin separation. This satisfies the physical requirements that $J_1(q)$ decrease with increasing $q$ and $J_1(0) < \overline{J}$, in order to be in the spin-glass phase. Our final results are not sensitive to this functional form provided $J_1(q) > 0$, for all $q$ of interest. We took $J_1(0)$ to be rather close to the maximum allowed value in order to obtain a sharp cusp in $\chi(0,T)$, as is observed experimentally. In Fig. 2 are shown the numerically computed curves $I(q,T)$ as a function of $T$ for several different values of $qa<1$. These curves illustrate the typical range of behavior for the calculated $I(q,T)$ and similar results have been obtained for very different model parameters. They should be viewed as qualitatively (rather than quantitatively) representative of the behavior of $I(q,T)$ in real spin-glasses. The dashed lines represent the "Bragg" contribution $I_B(q,T)$ whereas $T\chi(q,T)$ is plotted in the inset. The latter quantity always has a cusp at $T_c$. As in the experimental observations, $I(q,T)$ has a $q$-dependent maximum below $T_c$, which maximum increases toward $T_c$ (but always stays somewhat below it) as $q$ decreases. For small values of $q$ we also find a small feature at $T_c$ which may be a consequence of our mean-field calculations. In summary, these results corroborate the essential assumptions made in our data analysis.

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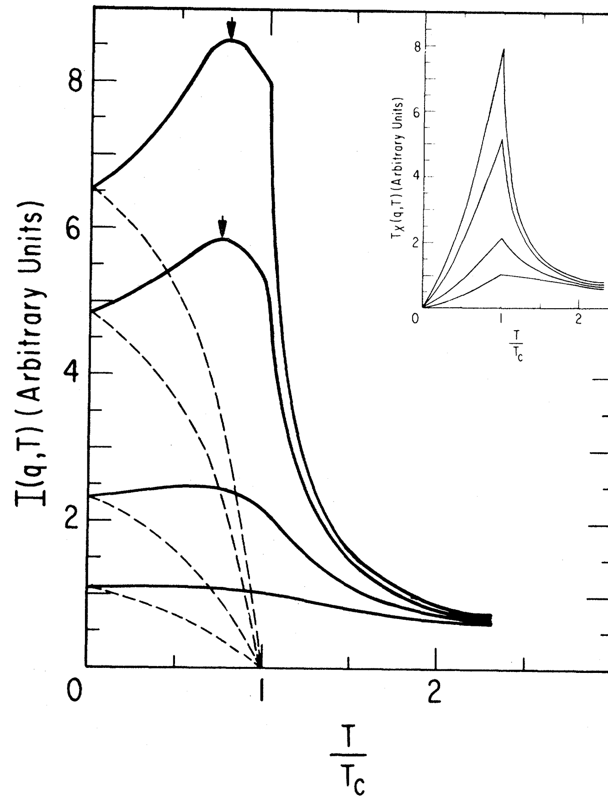


FIG. 2. Computed curves for $I(q,T)$ vs $T$ for $qa$ $=0.05$, 0.1, 0.2, 0.3 from top to bottom. The "Bragg" terms are dashed. The inset plots $T\chi(q,T)$.

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